

## ABSTRACT

Systems and methods related to the use of shape signatures for compactly representing molecular shape, and using shape signatures in both ligand-based and receptor-based molecular design. Ray-tracing is used to explore the volume interior to a ligand, or the space exterior to a receptor site. Shape signatures are then probability distributions derived from the ray-traces. Shape signatures can serve as compact descriptors of shape requiring modest storage space, and which may be quickly compared to test for shape similarity or complementarity.